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NEXAFS Investigations of Transition Metal Phosphide Catalysts

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Beamline(s): U1A

Introduction: Transition metal phosphides have recently emerged as a new type of hydroprocessing catalyst. These catalysts constitute a broad class of materials, which include MoP [1,2], WP [3], CoP, and Ni_2P [4]. The materials combine the refractory nature of ceramics with the conductive properties of metals, so are different from the transition metal sulfides. Work in this area is timely, as there is currently a pressing need to develop new types of catalysts that are more active than sulfides in order to meet stringent new specifications for sulfur content in transportation fuels. In this project the electronic structure of a series of reference phosphide samples are probed using NEXAFS spectroscopy with the intent of determining systematic trends that can be used to understand the properties of more complex materials.

Methods and Materials: The phosphides were prepared by the temperature-programmed reduction of phosphate precursors in a hydrogen stream. The precursors were obtained by combining metal salts and ammonium phosphate in stoichiometric proportions and calcining in air at 773 K. The reduction was carried out using linear ramps of 0.0167 K s^{-1} up to final temperatures of about 900 K. The resulting powders were passivated in a stream of 0.5 % O_2/He and stored until use.

Results: The NEXAFS spectra at the phosphorus L-edge of a series of compounds that included different metals such as MoP, WP, NbP, CoP, and Ni_2P, as well as different compositions like FeP, Fe_2P, and Fe_3P were obtained. The spectra were used as standards for supported materials like MoP/Al_2O_3 and Ni_2P/SiO_2. The figure below shows an example of such NEXAFS spectra. Currently the spectra are being analyzed to relate the spectral features to the structure of the compounds.

Conclusions: Standard spectra of reference compounds can be used to identify the presence of difference phases in supported catalysts.

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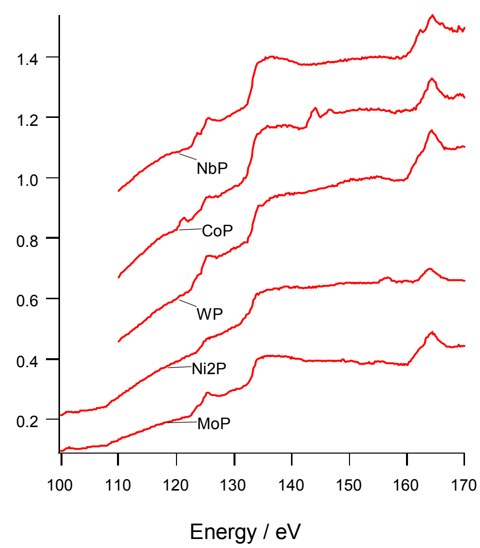

Figure 1. NEXAFS Spectra of Phosphides